Experimental FTIR-MI and Theoretical Studies of Isocyanic Acid Aggregates

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Streszczenie

Homoaggregates of isocyanic acid (HNCO) were studied using FTIR spectroscopy combined with a low-temperature matrix isolation technique and quantum chemical calculations. Computationally, the structures of the HNCO dimers and trimers were optimized at the MP2, B3LYPD3 and B2PLYPD3 levels of theory employing the 6-311++G(3df,3pd) basis set. Topological analysis of the electron density (AIM) was used to identify the type of non-covalent interactions in the studied aggregates. Five stable minima were located on the potential energy surface for $(HNCO)_2$, and nine were located on the potential energy surface for $(HNCO)_3$. The most stable dimer (D1) involves a weak, almost linear N-H···N hydrogen bond. Other structures are bound by a N-H···O hydrogen bond or by O···C or N···N van der Waals interactions. Similar types of interactions as in $(HNCO)_2$ were found in the case of HNCO trimers. Among nine stable $(HNCO)_3$ structures, five represent cyclic forms. The most stable T1 trimer structure is characterized by a six-membered ring formed by three N-H···N hydrogen bonds and representing high symmetry (C_{3h}). The analysis of the HNCO/Ar spectra after deposition indicates that the N-H···O hydrogen-bonded dimers are especially prevalent. Upon annealing, HNCO trimers were observed as well. Identification of the experimentally observed species relied on previous experimental data on HNCO complexes as well as computed data on HNCO homoaggregates' vibrational spectra.

Słowa kluczowe

HNCO, hydrogen bond, Fourier transform infrared (FTIR), matrix isolation (MI), solid argon, vibrational spectroscopy, intermolecular interaction, computational chemistry, molecular complex, atmospheric chemistry

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